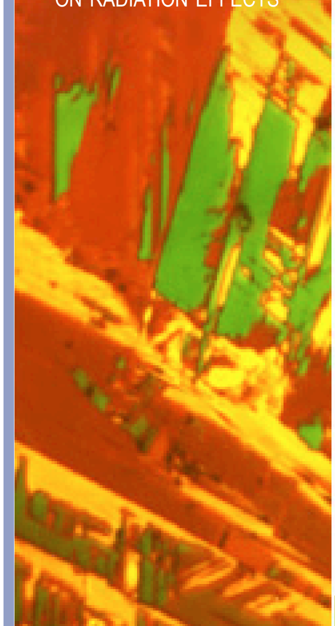
MST e NEWS

April 2012

INSIDE



Laboratory's materials research to be showcased at capability review

The world-record highest non-destructive magnetic field achieved last month at the National High Magnetic Field Laboratory-Pulsed Field Facility will be just one technical achievement featured during the 2012 Materials Capability Review.

From April 29 to May 2 scientists from 18 groups and 8 divisions will discuss their research in presentation and poster sessions at the Oppenheimer Study Center and the National High Magnetic Field Laboratory.

Organized by the Experimental Physical Sciences Directorate, the external peer review is designed to assess the quality of materials research and provide advice on technical contributions. This year's review will emphasize research in computational co-design for materials; high explosives and high pressure; high magnetic fields; and condensed matter physics.

Technical sessions begin Monday, April 30 at 8:30 a.m. when the review's technical host Materials Physics and Applications Division Leader Toni Taylor will present an overview of Materials at Los Alamos, including an update on an implementation plan for the Materials Strategy. She will be followed by MaRIE Capture Manager John Sarrao, who will discuss the latest developments related to the Laboratory's proposed flagship experimental facility for predicting and controlling materials in dynamic extremes.

For the 2012 Materials Capability Review, Gary Was of the University of Michigan returns to co-chair, with Barbara Jones of IBM Research-Almaden, a nine-member committee from universities, national laboratories, and research institutions. Theme leaders are Theoretical Division Leader Antonio Redondo, Weapons Experiments Division Leader David Funk, NHMFL-PFF Director Charles Mielke, and Condensed Matter & Magnet Science Group Leader Michael Hundley.

Members of the Laboratory's materials community are invited to attend. For the agenda, please see int.lanl.gov/org/padste/adeps/.

From Mark's Desk

As I write this Chris Stanek has just returned from Carlsbad where he spent a few days at the National Nuclear Fuel Cycle Summit (attended by Governor Susanna Martinez) and Ken McClellan has just left for Japan where he will cement an international collaboration with JAEA on oxidation in ceramic fuels. Also, I am pleased to welcome Stu Maloy back to MST Division after 2 years in the Civilian Nuclear Power program office. Since activity in the arena of materials for radiation applications is distributed across all four groups in MST (and indeed across PADSTE) it is possible to overlook its integrated impact, which is considerable. So in this "From the Desk" I thought I would take the opportunity to acknowledge the breadth of applied and fundamental studies of radiation effects in MST division, drawing attention to some recent wins and speculating on the future.

The range of funding sources that focus on radiation effects in MST reads like an alphabet soup: CASL, EFRC, NEAMS, FC R&D and LDRD. Much work is applied, initiated both by the Office of Nuclear Energy and by the NNSA, but there is considerable activity focusing on fundamental research funded by the Office of Science or by LDRD. The breadth of activity is considerable with examples that include measurement and prediction of the thermophysical properties of new compositions of ceramic fuels; development of new cladding coatings for improved accident tolerance; the use of supercomputers to connect first principles insights to engineering relevance; and non-destructive examination of welds removed from a commercial reactor pressure vessel.

As we consider future avenues of research it is worth remembering that the Office of Nuclear Energy is no less vulnerable (and perhaps more so) to the political winds du jour than any other department. Unsurprisingly, Fukushima has placed a premium on R&D that focuses on materials for accident tolerance or accident mitigation. This is evident from recent funding calls (which, co-incidentally also place a premium on industrial engagement). Nevertheless and despite the focus on accidents,

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the need for R&D relevant to the broader nuclear energy enterprise and radiation damage appears as strong as ever. Consider that 20 percent of the electricity in the United States continues to be produced by nuclear reactors. In the absence of a technological breakthrough that allows energy storage and movement of energy produced by renewables, nuclear will remain a significant part of baseload capacity (unless we abdicate control of CO_2 emissions). In passing, I would note that in March, the nuclear regulatory commission issued the first new licenses for two power reactors in more than a decade. Meanwhile NIF and ITER are billion dollar facility investments with the potential to place structural materials in unprecedented fusion regimes. Finally, the blue ribbon commission, which is responsible for making recommendations pertinent to the "back end of the nuclear fuel cycle" in addition to asserting that dry storage of used nuclear fuel is an interim solution, also advocated innovative R&D for long term solutions to the waste disposal problem (see www.brc.gov).

So, how is MST placed to respond to these opportunities? The good news is that we have a variety of staff that are influential in managing the NE R&D portfolio. On the experimental side, Ken McClellan and Stu Maloy are program leads in the Fuel Cycle R&D initiative focusing on fuel and cladding respectively. Dave Dombrowski is a program manager for the Convert Fuel Fabrication, a Non-Proliferation program in Global Security. Meanwhile Chris Stanek and David Andersson are leaders in the CASL and NEAMS projects respectively, which complement the experiments with modeling and simulation. Our facilities are well aligned with future needs and we have been capitalizing on the unique skills at LANL. One good example is expertise in handling radioactive material in facilities such as Sigma or in the Electron Microscopy Laboratory that allows examination of (some) radioactive materials. Tarik Saleh (MST-16) uses the hot cells in CMR wing 9 to examine highly radioactive material removed from reactors.

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In situ monitoring of dynamic phenomena during solidification

The creation of microstructures by design with application-tailored properties requires directed synthesis and processing. Los Alamos scientists and collaborators are developing methods to monitor dynamic phenomena directly during phase transformations at non-ambient temperatures using novel imaging techniques. This will enable control of microstructure evolution, will allow for the validation and advancement of science-based theories, and will enable predictive model development over the length scale relevant for phase transformations and microstructure evolution.

Metallurgy (MST-6) and the Proton Radiography team completed the first in situ examinations of melting and solidification in aluminum-indium, gallium bismuth, tin-bismuth, and aluminum-copper alloys using 800-MeV proton radiography (pRad). Proton radiography, a unique capability at the Los Alamos Neutron Science Center (LANSCE), probes dynamic material phenomena. In this new application of pRad for materials studies, the researchers imaged heating and cooling of bulk metal alloy sections ranging from 2-6 mm in thickness (see Figure A). These images highlight liquid-liquid phase separation at elevated temperatures and solid-liquid interface movement. Advantages of proton radiography for these experiments include: time-resolved imaging of dynamic phenomena (e.g., localized fluid flow and solute segregation during solidification) and microstructure evolution, examination of a large field of view in millimeter thick samples (relevant to casting) that enables bulk materials analysis, and the ability to examine high density materials.

The scientists also monitored alloy melting and solidification using synchrotron x-ray radiography at Argonne National Laboratory's Advanced Photon Source. Figure B shows example radiographs captured just after continuous heating and slow or fast cooling of a 100 micron thick aluminum-copper (Al-Cu) sample. The images reveal that the cooling rate influences the length scale of the microstructure. Synchrotron x-ray radiography affords 1-2 micron spatial resolution. The post- mortem solidification microstructure of an Al-Cu alloy shown at the far right in Figure B was obtained using x-ray tomography at LANL. This image highlights the wealth of information about 3D microstructure evolution during processing that will be possible with in situ imaging techniques.

This work demonstrates that proton radiography and synchrotron x-ray radiography are complementary techniques for in situ observations and control of solidification behavior and microstructure evolution. The in situ methods will enable tomographic studies of 3D microstructure evolution during

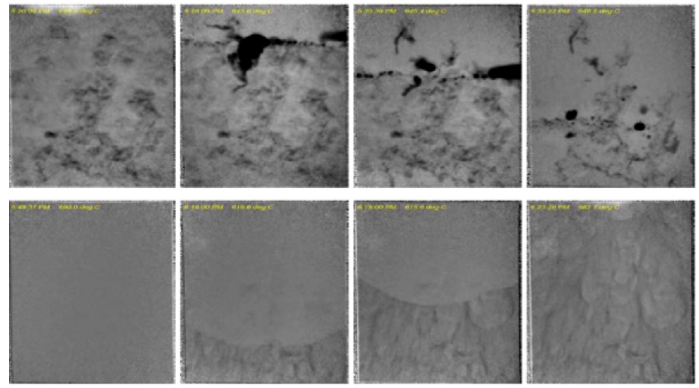

Figure A. Example time-resolved pRad images obtained during melting from the top downward (upper row images) and directional solidification from the bottom upward (lower row images) of a bulk 6 mm thick aluminum-indium (Al-In) sample. The field of view is approximately 44 x 44 mm^2. The darker regions observed during melting are indium-rich liquid, consistent with the liquid-liquid phase separation anticipated at elevated temperatures for this alloy system.

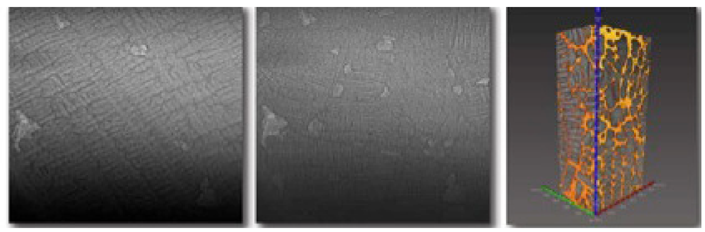

Figure B. Synchrotron x-ray radiography images obtained during continuous heating and slow cooling (left) or continuous heating and fast cooling (center) of a 100-micron thick aluminum-copper sample. The light, branched structures in the radiographs correspond to aluminum-rich dendrites. The field of view is approximately 1.4 x 1.4 mm2. A post-mortem x-ray tomography result (far right) of an Al-Cu alloy highlights the three-dimensional nature of the dendritic (gray) and interdendritic (orange) regions. The volume is approximately 0.7 x 1.1 x 2.4 mm^3.

processing. The monitoring techniques will help to achieve transformational advances in the creation of microstructures by design, which has been identified as a key grand challenge for synthesis and processing materials science. Moreover, this work will help to define key MaRIE capabilities needed for future process-aware solidification studies at LANL.

Researchers include Amy Clarke, Jason Cooley, Tim Tucker, Robert Field, Robert Aikin, David Korzekwa, Duncan Hammon, Kester Clarke, Jim Foley, Ralph Trujillo, Steve Quintana, Patrick Kennedy, Bo Folks, Tim Beard, Tyler Wheeler, Rick Hudson, Randy Edwards, Mark Paffett, J.D. Montalvo, Ann Kelly, and Dane Knowlton (MST-6); Paul Dunn (MST-6, now Intelligence Analysis and Technology, IAT-DO); Thomas Ott, Joshua Hill, Martha Barker, Finian O'Neill, and Megan Emigh (MST-6 summer students); Frank Merrill, Brian Hollander, Chris Morris, Fesseha Mariam, Carter Munson, and the Proton Radiography Team (Neutron Science and Technology, P-23 and Subatomic Physics, P-25); Marshall Maez (Prototype Fabrication – Fabrication Services, PF-FS); Brian Patterson

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Monitoring . . (Polymers and Coatings, MST-7); David Teter (Materials Science and Technology, MST-DO), Dan Thoma (Institutes, INST-OFF), Wah-Keat Lee (Brookhaven National Laboratory); Kamel Fezzaa and Alex Deriy (Argonne National Laboratory). Laboratory Directed Research and Development (LDRD) funded this Materials in Extremes/MaRIE-related project. The research supports the Lab's Energy Security and Nuclear Deterrence mission areas and the Materials for the Future and Science of Signatures science pillars.

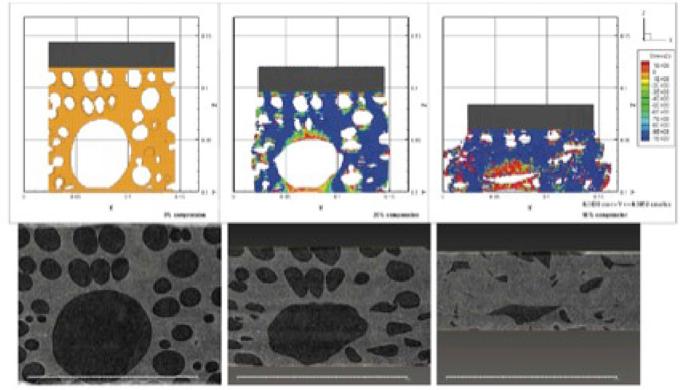
Technical contact: Amy Clarke

Comparison of in situ 3D imaged foams in compression with modeling

The ability to predict the performance of materials under dynamic or repeated dynamic load is paramount for lifetime prediction in certain applications. Brian M. Patterson, Kevin Henderson, and Zachary Smith (MST-7); Duan Zhang and Paul Giguere (Fluid Dynamics and Solid Mechanics, T-3) have demonstrated the power of using experimentally imaged three-dimensional (3D) data, fed into a material point method (MPM) modeling code, to better understand the performance of foams during in situ measurements. The experiments can be used to validate the models in a state-of-the-art code, which in turn will provide a theoretical basis for the experimental results and a reliable predictive capability of a material's performance. The journal *Microscopy and Analysis* will publish the research.

Foamed polysiloxane rubbers have numerous industrial applications that require load-bearing properties to be retained over long service lives. Because the installed materials may be difficult to monitor directly, the predictive value of modeling can be significant. The correct foam for an application must have the appropriate chemical formulation, bulk density, and resistance to age-related loss of performance.

Micro X-ray computed tomography (μXCT) creates a digital 3D image of a material based upon its X- ray attenuation properties. A series of radiographs are collected as the sample is rotated a minimum of 180°. These images are then reconstructed into a 3D image of the sample. These digital 3D images are very useful in understanding the morphology, as well as morphological changes, as a result of experiment. The researchers used an Xradia micro x-ray computed tomography instrument with a Deben compression cell to image cylinders of polysiloxane rubber foam at various percentages of compression. Coupling this capability to a 3D image analysis software package enables measurement of morphological changes of the material. The scientists can measure the percent void volume as a function of compression, as well as changes in



Approximately the same slices through the modeled (top) and experimentally (bottom) compressed foam at 0, ~20, and ~50% compression. The scale bar on the bottom is 1.2 mm. Color in the modeled data is stress. There is good agreement on the deformation of the large void.

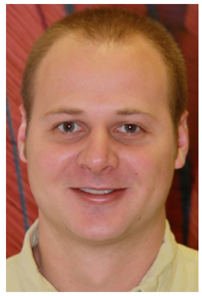
the void structure. Typical void statistics acquired include surface area, Feret Shape (3D measure of the aspect ratio), and many others. Each void can be measured individually as a function of the compressive load. With this method, lot-to-lot and in situ morphological changes can be quantified rigorously.

MPM modeling, used for modeling large deformations, becomes even more robust when modeling from an experimentally derived data set. The researchers binned down the initial dataset of uncompressed data to a 100 x 100 x 100 voxel (volume pixel) cube to be fed into the MPM model. They did not adjust material parameters in their first try. The scientists used the MPM in the LANL-developed CartaBlanca code to simulate the foam material under uniaxial compression. Their main goal was to demonstrate that the code is capable of handling large deformation and complex irregular geometry of a material that contains voids of various shapes. A comparison of the 3D images of the in situ compressed foam with the MPM modeled foam shows good agreement in the morphological changes to the foam structure (see figure). Feeding the initial state images and their statistics into an advanced numerical simulation code that is based on MPM adds a level of rigor to the modeling process that was not possible until now.

NNSA Campaign 2 (Rick Martineau, LANL program manager) and the Enhanced Surveillance Campaign (Tom Zocco, LANL program manager) funded the research. The work supports the Lab's Nuclear Deterrence mission area and the Materials for the Future science pillar.

Technical contact: Brian Patterson

John Carpenter to receive TMS Young Leader Professional Development Award



The Minerals, Metals and Materials Society (TMS) has selected John Carpenter (MST-6 and Center for Integrated Nanotechnologies, MPA-CINT) to receive the 2012 TMS Extraction and Processing Division Young Leader Professional Development Award.

The Society created the annual award to enhance the professional development of dynamic young people from TMS's five technical divisions. Awardees participate in Society activities, attend TMS conferences, network with Society members and leaders, receive mentoring from TMS division leaders, and serve as judges for division-sponsored student events at the TMS Annual Meeting.

Carpenter earned a doctorate in Materials Science and Engineering at the Ohio State University. He joined LANL in 2010 as a postdoctoral researcher in MST-6 and MPA-CINT. His research on the bulk fabrication and characterization of bimetallic laminar nanocomposites is associated with a LANL Energy Frontier Research Center (Center for Materials at Irradiation and Mechanical Extremes) and the Laboratory Directed Research and Development (LDRD) project, "Innovative and Validated Sub-micron to Mesoscale Modeling of the Evolution of Interface Structure and Properties under Extreme Strains." He serves as the communications chair for the Los Alamos Postdoctoral Association.

Carpenter is a member of the Nanomechanical Behavior and the Mechanical Behavior of Materials Organizing Committees for TMS. In addition, he is a member, session organizer, and the Journal of Minerals, Metals, and Materials representative for the Materials Characterization Organizing Committee for TMS.

The Minerals, Metals & Materials Society (TMS) is an international professional organization of nearly 10,000 members, encompassing the entire range of materials and engineering, from minerals processing and primary metals production to basic research and the advanced applications of materials.

Scientific journal publishes special issue in honor of Carlos Tomé

The journal *Modelling and Simulation in Materials Science and Engineering* published a special issue in honor of Carlos Tomé (Materials Science in Radiation and Dynamics Extremes, MST-8) and his contributions to the field of mechanical behavior of polycrystalline materials. The special issue featured ten papers that were presented at a symposium on the occasion of his 60th birthday. From March to August 31, the journal will offer free access to the papers, which are a sampling of the different length-scales, materials, and experimental and modeling techniques addressed in the symposium. Tomé has a doctorate in Physics from the National University of La Plata, Argentina. He joined LANL in 1996 and serves as the MST-8 materials modeling team leader. Ricardo A. Lebensohn (MST-8) co-organized the symposium and served as guest editor of the journal's special issue. The original invited talks were delivered at the 2011 TMS (The Minerals, Metals and Materials Society) Annual Meeting and Exhibition in San Diego, CA. The symposium featured more than 90 presentations, including a keynote by Tomé, and 35 invited lectures.

"Throughout his career, Dr. Tomé has pioneered the theoretical and numerical development of models of polycrystal mechanical behavior, with emphasis on the role played by texture and microstructure on the anisotropic behavior of engineering materials," Lebensohn wrote in the preface of the special issue. "His many contributions have been critical in establishing a strong connection between models and experiments, and in bridging different scales in the pursuit of robust multiscale models with experimental integration."

Reference: Special Issue: Polycrystal Modelling with Experimental Integration: A Symposium Honoring Carlos Tomé, *Modelling and Simulation in Materials Science and Engineering* **20** (2), 020201 (2012).

Technical contact: Ricardo Lebensohn

Celebrating service

Congratulations to the following MST Division employees celebrating service anniversaries this month:

Roland Schulze, MST 6	20 years
Lily Wang, MST-6	20 years
Stephen Gravener, MST-6	10 years
Dennis Guidry, MST-6	10 years
Anders Andersson, MST-8	5 years

Desk . . New facilities include the Fuels Research Laboratory where Andy Nelson (MST-7) measures thermophysical properties and assesses fabrication processes for urania based fuels. In the Ion Beam Materials Laboratory Yong Wang, Magda Caro (MST-8) and Peter Hosemann (UCB) recently installed new capability to allow ion irradiation of a surface in contact with molten metal to assess whether there are synergistic effects of irradiation on corrosion rate. This complements activity at LANSCE where the DELTA loop (a testbed for cooling systems relevant to future spallation neutron sources like MTS) has recently been restarted. This work is relevant to the current interest in Small Modular Reactors and to startup companies such as Hyperion or Terrapower. In a parallel initiative, also at the IBML, Ming Tang and Marilyn Hawley have implemented a dual beam irradiation system whereby two species can be implanted simultaneously. This allows research on whether sequential or simultaneous ion beam irradiations produce different results, which is crucial to the question of whether ions can be used for accelerated simulation of damage in reactor environments.

Underpinning the facility investments, fundamental research activity spans the atomistic to macroscopic regime. To mention a few examples: Blas Uberuaga with Amit Misra is examining the effects of interfaces; Alfredo Caro is examining the radiation resistance of nanofoams; and Don Brown is using the advanced photon source to make 3D nondestructive maps of grain morphology and performing micron scale tomography measurements on centimeter scale urania fuel pellets. Researchers in MST are hosting international conferences in Santa Fe this spring pertaining to the study of radiation effects (see sidebar).

In conclusion, our underlying strategy in MST focuses on the physics and chemistry that govern performance. This "science-based" approach maximizes the applicability of the insights to the broadest set of problems and will be articulated in the section of the materials strategy focusing on radiation extremes due soon. Radiation environments, and the challenge of designing materials that can survive them, lie at the center of the prevailing "extreme conditions" and "mesoscale" zeitgeist. Atomistic studies using supercomputers coupled with the promise of exascale computing hold tantalizing hints that insights from first principles calculations of radiation damage can be ported to the macroscale. These are areas of research that MST Division is well placed to leverage and embody the "materials by design" paradigm implicit in MaRIE. So even if the nuclear renaissance is currently slowed, R&D for the nuclear enterprise is likely alive and well in MST for the foreseeable future.

MST-8 Deputy Group Leader Mark Bourke

Three spring meetings on radiation effects

To promote interaction between communities with mutual interests, MST staff (Stanek, Uberuaga, and Caro) are hosting three joint international meetings in Santa Fe focused on radiation damage and defects in materials.

The 2012 Computer Simulation of Radiation Effects in Solids (11th edition) is a biennial conference focusing on advanced computer modeling of surface and bulk phenomena stimulated by all forms of irradiation. Fundamental understanding of these phenomena is often not accessible by experiments, since they occur on very small time and length scales. A vigorous development of both computer hardware and theoretical methodologies that has occurred in recent years has pushed the field into the forefront of a modern science.

The International Conference on Defects in Insulating Materials is the 18th edition of a series that began in 1956 at Argonne with the meeting "Color Centers in Alkali Halides." The conference takes place every four years alternating with Europe-specific conferences (EURODIM). The series provides a broad international forum on the science and technology of defect-related phenomena in crystalline and amorphous wide band-gap materials, with focus on both experiment and theory.

Both conferences will be held concurrently June 24-29.

Just before the two conferences, on June 22-24, the MatGen-IV School on Frontiers of Computational Materials Science meeting is intended for graduate students, postdoctoral researchers, and researchers interested on having an up-to-date overview of current active research subjects in the field of computational materials science. It will center on two topics: Beyond Molecular Dynamics: Long Time Atomic-Scale Simulations and Non-adiabatic electrons: beyond the Born-Oppenheimer approximation.

For more information, please see:
COSIRES: cosires.newmexicoconsortium.org/
ICDIM: icdim.newmexicoconsortium.org/
MATGEN-IV: www.matgen-iv.org/

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